Nitrogen-Linked Diphosphine Ligands with Ethers Attached to Nitrogen for Chromium Catalyzed Ethylene Tri- and Tetramerizations

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S1. Structural drawings, tables with structural parameters, and crystallographic information for **5**.

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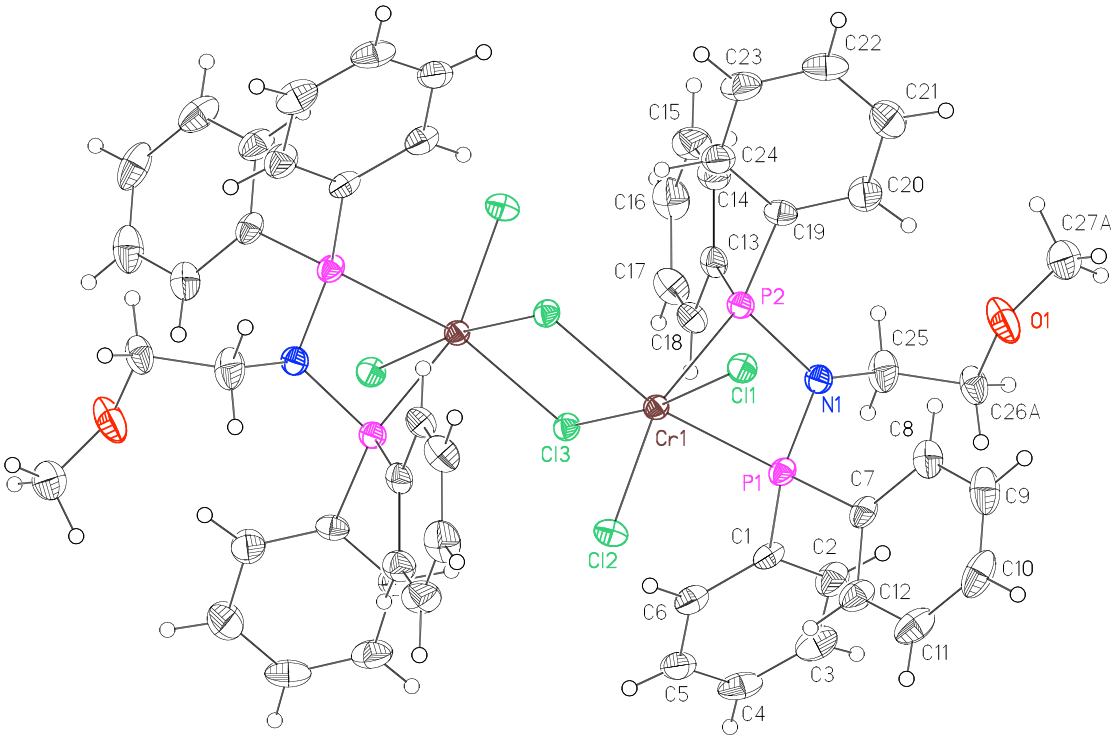

Figure 1. Structural drawing of **5** with thermal ellipsoids at the 50% probability level.

Table 1. Crystal data and structure refinement for 5 (CCDC 258068).

Empirical formula	$C_{54}H_{54}Cl_6N_2O_2P_4Cr_2 \bullet 4(CH_2Cl_2)$
Formula weight	1543.28
Crystallization Solvent	Dichloromethane/petroleum ether
Crystal Habit	Block
Crystal size	0.41 x 0.16 x 0.15 mm^3
Crystal color	Sapphire blue

Data Collection

Type of diffractometer	Bruker SMART 1000
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 19148 reflections used in lattice determination	2.19 to 33.48°
Unit cell dimensions	a = 11.3376(5) Å b = 18.5701(7) Å β= 108.7220(10)° c = 16.7264(7) Å
Volume	3335.2(2) $Å^3$
Z	2
Crystal system	Monoclinic
Space group	$P2_1/n$
Density (calculated)	1.537 Mg/m^3
F(000)	1572
θ range for data collection	1.69 to 33.74°
Completeness to θ = 33.74°	90.1 %
Index ranges	$-16 \le h \le 16, -28 < k < 28, -25 < l < 25$
Data collection scan type	ω scans at 3 ϕ settings of 2θ=-28° and 2 at 2θ=-40°

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Reflections collected	54219
Independent reflections	12015 [R_{int}= 0.0669]
Absorption coefficient	1.026 mm^{-1}
Absorption correction	None
Max. and min. transmission	0.8614 and 0.6785
Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Difference Fourier map
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	12015 / 0 / 491
Treatment of hydrogen atoms	Unrestrained, disordered riding
Goodness-of-fit on F^2	1.596
Final R indices [I>2σ(I), 7974 reflections]	R1 = 0.0458, *w*R2 = 0.0749
R indices (all data)	R1 = 0.0776, *w*R2 = 0.0783
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.002
Average shift/error	0.000
Largest diff. peak and hole	1.183 and -0.759 e.$Å^{-3}$

Special Refinement Details

There is disorder in the methyl-ethyl keytone ligand attached to nitrogen. The disorder was modeled with alternate positions for the ethyl carbon atom alpha to oxygen (C26A & B) with the corresponding changes in the methyl carbon (C27A & B). The oxygen atom (O1) was refined at a single position. The molecule sits on a center of symmetry, therefore, only the unique atoms are labeled in the figures. Disorder is also observed in the dichloromethane solvents (not shown in the figures).

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 5 (CCDC 258068). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}	Occ
Cr(1)	10258(1)	5437(1)	9145(1)	16(1)	1
Cl(1)	9270(1)	6364(1)	8313(1)	21(1)	1
Cl(2)	11971(1)	6091(1)	9890(1)	23(1)	1
Cl(3)	11000(1)	4392(1)	9962(1)	18(1)	1
P(1)	11095(1)	5139(1)	8022(1)	19(1)	1
P(2)	8871(1)	4635(1)	8053(1)	18(1)	1
O(1)	8632(1)	4810(1)	5551(1)	42(1)	1
N(1)	9828(1)	4661(1)	7445(1)	20(1)	1
C(1)	12508(2)	4597(1)	8274(1)	20(1)	1
C(2)	12868(2)	4222(1)	7671(2)	30(1)	1
C(3)	13952(2)	3818(1)	7916(2)	34(1)	1
C(4)	14698(2)	3807(1)	8740(2)	32(1)	1
C(5)	14381(2)	4191(1)	9333(2)	28(1)	1
C(6)	13280(2)	4581(1)	9109(1)	26(1)	1
C(7)	11338(2)	5868(1)	7377(1)	22(1)	1
C(8)	10389(2)	6115(1)	6669(1)	29(1)	1
C(9)	10589(2)	6705(1)	6231(2)	37(1)	1
C(10)	11706(2)	7060(1)	6487(2)	37(1)	1
C(11)	12635(2)	6838(1)	7192(2)	34(1)	1
C(12)	12458(2)	6242(1)	7641(2)	29(1)	1
C(13)	8569(2)	3684(1)	8144(1)	21(1)	1
C(14)	7365(2)	3413(1)	7947(1)	27(1)	1
C(15)	7165(2)	2691(1)	8037(2)	33(1)	1
C(16)	8149(2)	2226(1)	8309(2)	36(1)	1
C(17)	9354(2)	2485(1)	8501(1)	30(1)	1
C(18)	9564(2)	3203(1)	8424(1)	24(1)	1
C(19)	7343(2)	5008(1)	7514(1)	21(1)	1
C(20)	6889(2)	5165(1)	6672(2)	33(1)	1
C(21)	5683(2)	5441(1)	6328(2)	39(1)	1
C(22)	4971(2)	5564(1)	6842(2)	34(1)	1
C(23)	5430(2)	5418(1)	7683(2)	33(1)	1
C(24)	6614(2)	5135(1)	8024(2)	28(1)	1
C(25)	9770(2)	4142(1)	6756(1)	32(1)	1
C(26A)	9747(3)	4423(2)	5930(2)	29(1)	0.606(4)
C(27A)	7688(4)	4691(2)	4830(2)	46(1)	0.606(4)
C(26B)	8771(5)	4127(3)	6040(3)	28(1)	0.394(4)
C(27B)	8508(6)	5082(3)	4772(4)	38(2)	0.394(4)
C(31)	3736(2)	2840(1)	5658(2)	41(1)	1
Cl(11)	4592(1)	3648(1)	5838(1)	53(1)	1
Cl(12)	2282(4)	2929(2)	5855(3)	43(1)	0.54(2)
Cl(13)	2215(5)	3022(5)	5595(12)	90(2)	0.46(2)
C(32)	3105(2)	2924(2)	1044(2)	52(1)	1
Cl(21)	4595(1)	2819(1)	976(1)	49(1)	1
Cl(22)	1989(2)	2464(3)	290(4)	55(1)	0.551(12)
Cl(23)	2129(3)	2175(4)	548(2)	64(1)	0.449(12)

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Table 3. Selected bond lengths [Å] and angles [°] for 5 (CCDC 258068).

Cr(1)-Cl(1)	2.2701(5)	Cl(2)-Cr(1)-Cl(3)#1	99.259(19)
Cr(1)-Cl(2)	2.2900(5)	Cl(3)-Cr(1)-Cl(3)#1	85.488(17)
Cr(1)-Cl(3)	2.3679(5)	Cl(1)-Cr(1)-P(1)	86.376(19)
Cr(1)-Cl(3)#1	2.3939(5)	Cl(2)-Cr(1)-P(1)	93.90(2)
Cr(1)-P(1)	2.4251(6)	Cl(3)-Cr(1)-P(1)	96.036(18)
Cr(1)-P(2)	2.4862(6)	Cl(3)#1-Cr(1)-P(1)	166.69(2)
Cl(3)-Cr(1)#1	2.3939(5)	Cl(1)-Cr(1)-P(2)	86.157(19)
		Cl(2)-Cr(1)-P(2)	160.56(2)
Cl(1)-Cr(1)-Cl(2)	95.553(19)	Cl(3)-Cr(1)-P(2)	87.510(18)
Cl(1)-Cr(1)-Cl(3)	171.71(2)	Cl(3)#1-Cr(1)-P(2)	100.090(18)
Cl(2)-Cr(1)-Cl(3)	92.196(19)	P(1)-Cr(1)-P(2)	66.837(18)
Cl(1)-Cr(1)-Cl(3)#1	90.364(18)	Cr(1)-Cl(3)-Cr(1)#1	94.511(17)

Symmetry transformations used to generate equivalent atoms: #1 -x+2,-y+1,-z+2

Table 4. Bond lengths [Å] and angles [°] for 5 (CCDC 258068).

Cr(1)-Cl(1)	2.2701(5)	C(10)-C(11)	1.368(3)
Cr(1)-Cl(2)	2.2900(5)	C(10)-H(10A)	0.93(2)
Cr(1)-Cl(3)	2.3679(5)	C(11)-C(12)	1.387(3)
Cr(1)-Cl(3)#1	2.3939(5)	C(11)-H(11A)	0.88(2)
Cr(1)-P(1)	2.4251(6)	C(12)-H(12A)	0.92(2)
Cr(1)-P(2)	2.4862(6)	C(13)-C(14)	1.391(3)
Cl(3)-Cr(1)#1	2.3939(5)	C(13)-C(18)	1.397(3)
P(1)-N(1)	1.7010(16)	C(14)-C(15)	1.377(3)
P(1)-C(7)	1.8058(19)	C(14)-H(14A)	0.89(2)
P(1)-C(1)	1.8231(18)	C(15)-C(16)	1.367(3)
P(2)-N(1)	1.7089(15)	C(15)-H(15A)	0.91(2)
P(2)-C(19)	1.8141(18)	C(16)-C(17)	1.385(3)
P(2)-C(13)	1.8147(19)	C(16)-H(16A)	0.97(2)
O(1)-C(27A)	1.350(4)	C(17)-C(18)	1.369(3)
O(1)-C(27B)	1.361(6)	C(17)-H(17A)	0.87(2)
O(1)-C(26A)	1.415(3)	C(18)-H(18A)	0.855(18)
O(1)-C(26B)	1.491(5)	C(19)-C(20)	1.367(3)
N(1)-C(25)	1.488(2)	C(19)-C(24)	1.385(3)
C(1)-C(6)	1.390(3)	C(20)-C(21)	1.399(3)
C(1)-C(2)	1.391(3)	C(20)-H(20A)	0.88(2)
C(2)-C(3)	1.385(3)	C(21)-C(22)	1.373(3)
C(2)-H(2A)	0.89(2)	C(21)-H(21A)	0.92(2)
C(3)-C(4)	1.365(3)	C(22)-C(23)	1.361(3)
C(3)-H(3A)	0.84(2)	C(22)-H(22A)	0.89(2)
C(4)-C(5)	1.361(3)	C(23)-C(24)	1.383(3)
C(4)-H(4A)	0.86(2)	C(23)-H(23A)	0.86(2)
C(5)-C(6)	1.387(3)	C(24)-H(24A)	0.92(2)
C(5)-H(5A)	0.841(19)	C(25)-C(26B)	1.359(5)
C(6)-H(6A)	0.906(19)	C(25)-C(26A)	1.468(4)
C(7)-C(12)	1.389(3)	C(25)-H(25A)	0.9900
C(7)-C(8)	1.397(3)	C(25)-H(25B)	0.9900
C(8)-C(9)	1.376(3)	C(25)-H(25C)	0.9900
C(8)-H(8A)	0.91(2)	C(25)-H(25D)	0.9901
C(9)-C(10)	1.370(3)	C(26A)-H(25C)	1.2145
C(9)-H(9A)	0.86(2)	C(26A)-H(26A)	0.9900

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C(26A)-H(26B)	0.9900	C(26A)-O(1)-C(26B)	53.0(2)
C(27A)-H(27A)	0.9800	C(25)-N(1)-P(1)	126.65(13)
C(27A)-H(27B)	0.9800	C(25)-N(1)-P(2)	124.37(13)
C(27A)-H(27C)	0.9800	P(1)-N(1)-P(2)	105.01(8)
C(26B)-H(26C)	0.9900	C(6)-C(1)-C(2)	118.74(18)
C(26B)-H(26D)	0.9900	C(6)-C(1)-P(1)	117.86(15)
C(27B)-H(27D)	0.9800	C(2)-C(1)-P(1)	123.37(16)
C(27B)-H(27E)	0.9800	C(3)-C(2)-C(1)	119.7(2)
C(27B)-H(27F)	0.9800	C(3)-C(2)-H(2A)	120.5(14)
C(31)-Cl(13)	1.726(7)	C(1)-C(2)-H(2A)	119.8(14)
C(31)-Cl(11)	1.760(2)	C(4)-C(3)-C(2)	120.7(2)
C(31)-Cl(12)	1.789(5)	C(4)-C(3)-H(3A)	123.7(17)
C(31)-H(31A)	0.9900	C(2)-C(3)-H(3A)	115.6(17)
C(31)-H(31B)	0.9900	C(5)-C(4)-C(3)	120.3(2)
C(31)-H(31C)	0.9901	C(5)-C(4)-H(4A)	117.8(16)
C(31)-H(31D)	0.9899	C(3)-C(4)-H(4A)	121.8(16)
C(32)-Cl(22)	1.701(3)	C(4)-C(5)-C(6)	120.2(2)
C(32)-Cl(21)	1.741(2)	C(4)-C(5)-H(5A)	124.4(13)
C(32)-Cl(23)	1.804(5)	C(6)-C(5)-H(5A)	115.3(13)
C(32)-H(32A)	0.9900	C(5)-C(6)-C(1)	120.3(2)
C(32)-H(32B)	0.9900	C(5)-C(6)-H(6A)	120.2(12)
C(32)-H(32C)	0.9899	C(1)-C(6)-H(6A)	119.5(12)
C(32)-H(32D)	0.9899	C(12)-C(7)-C(8)	118.79(19)
		C(12)-C(7)-P(1)	118.95(15)
Cl(1)-Cr(1)-Cl(2)	95.553(19)	C(8)-C(7)-P(1)	121.93(16)
Cl(1)-Cr(1)-Cl(3)	171.71(2)	C(9)-C(8)-C(7)	120.0(2)
Cl(2)-Cr(1)-Cl(3)	92.196(19)	C(9)-C(8)-H(8A)	121.1(13)
Cl(1)-Cr(1)-Cl(3)#1	90.364(18)	C(7)-C(8)-H(8A)	118.6(13)
Cl(2)-Cr(1)-Cl(3)#1	99.259(19)	C(10)-C(9)-C(8)	120.7(2)
Cl(3)-Cr(1)-Cl(3)#1	85.488(17)	C(10)-C(9)-H(9A)	120.3(14)
Cl(1)-Cr(1)-P(1)	86.376(19)	C(8)-C(9)-H(9A)	119.0(15)
Cl(2)-Cr(1)-P(1)	93.90(2)	C(11)-C(10)-C(9)	120.2(2)
Cl(3)-Cr(1)-P(1)	96.036(18)	C(11)-C(10)-H(10A)	120.3(15)
Cl(3)#1-Cr(1)-P(1)	166.69(2)	C(9)-C(10)-H(10A)	119.5(14)
Cl(1)-Cr(1)-P(2)	86.157(19)	C(10)-C(11)-C(12)	120.1(2)
Cl(2)-Cr(1)-P(2)	160.56(2)	C(10)-C(11)-H(11A)	122.6(14)
Cl(3)-Cr(1)-P(2)	87.510(18)	C(12)-C(11)-H(11A)	117.2(14)
Cl(3)#1-Cr(1)-P(2)	100.090(18)	C(11)-C(12)-C(7)	120.2(2)
P(1)-Cr(1)-P(2)	66.837(18)	C(11)-C(12)-H(12A)	121.3(13)
Cr(1)-Cl(3)-Cr(1)#1	94.511(17)	C(7)-C(12)-H(12A)	118.3(13)
N(1)-P(1)-C(7)	108.42(9)	C(14)-C(13)-C(18)	118.30(18)
N(1)-P(1)-C(1)	111.23(8)	C(14)-C(13)-P(2)	121.98(15)
C(7)-P(1)-C(1)	105.09(8)	C(18)-C(13)-P(2)	119.72(14)
N(1)-P(1)-Cr(1)	95.11(5)	C(15)-C(14)-C(13)	120.7(2)
C(7)-P(1)-Cr(1)	117.67(6)	C(15)-C(14)-H(14A)	120.9(13)
C(1)-P(1)-Cr(1)	118.70(6)	C(13)-C(14)-H(14A)	118.4(13)
N(1)-P(2)-C(19)	112.39(8)	C(16)-C(15)-C(14)	120.4(2)
N(1)-P(2)-C(13)	104.47(8)	C(16)-C(15)-H(15A)	121.3(13)
C(19)-P(2)-C(13)	103.70(9)	C(14)-C(15)-H(15A)	118.2(13)
N(1)-P(2)-Cr(1)	92.76(5)	C(15)-C(16)-C(17)	119.8(2)
C(19)-P(2)-Cr(1)	114.48(6)	C(15)-C(16)-H(16A)	121.7(12)
C(13)-P(2)-Cr(1)	127.84(6)	C(17)-C(16)-H(16A)	118.5(12)
C(27A)-O(1)-C(27B)	52.9(3)	C(18)-C(17)-C(16)	120.4(2)
C(27A)-O(1)-C(26A)	130.9(3)	C(18)-C(17)-H(17A)	118.1(14)
C(27B)-O(1)-C(26A)	114.9(3)	C(16)-C(17)-H(17A)	121.5(14)
C(27A)-O(1)-C(26B)	105.3(3)	C(17)-C(18)-C(13)	120.5(2)
C(27B)-O(1)-C(26B)	143.2(3)	C(17)-C(18)-H(18A)	119.8(12)

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C(13)-C(18)-H(18A)	119.6(12)	O(1)-C(27A)-H(27B)	109.5
C(20)-C(19)-C(24)	119.72(19)	O(1)-C(27A)-H(27C)	109.5
C(20)-C(19)-P(2)	125.29(15)	C(25)-C(26B)-O(1)	112.2(4)
C(24)-C(19)-P(2)	114.99(16)	C(25)-C(26B)-H(26C)	109.2
C(19)-C(20)-C(21)	119.8(2)	O(1)-C(26B)-H(26C)	109.2
C(19)-C(20)-H(20A)	125.4(14)	C(25)-C(26B)-H(26D)	109.2
C(21)-C(20)-H(20A)	114.9(14)	O(1)-C(26B)-H(26D)	109.2
C(22)-C(21)-C(20)	119.8(2)	H(26C)-C(26B)-H(26D)	107.9
C(22)-C(21)-H(21A)	124.8(14)	O(1)-C(27B)-H(27D)	109.5
C(20)-C(21)-H(21A)	115.3(14)	O(1)-C(27B)-H(27E)	109.5
C(23)-C(22)-C(21)	120.5(2)	H(27D)-C(27B)-H(27E)	109.5
C(23)-C(22)-H(22A)	118.4(14)	O(1)-C(27B)-H(27F)	109.5
C(21)-C(22)-H(22A)	121.1(14)	H(27D)-C(27B)-H(27F)	109.5
C(22)-C(23)-C(24)	120.0(2)	H(27E)-C(27B)-H(27F)	109.5
C(22)-C(23)-H(23A)	121.1(16)	Cl(13)-C(31)-Cl(11)	109.2(3)
C(24)-C(23)-H(23A)	118.8(16)	Cl(11)-C(31)-Cl(12)	112.35(16)
C(23)-C(24)-C(19)	120.2(2)	Cl(13)-C(31)-H(31A)	122.6
C(23)-C(24)-H(24A)	119.6(14)	Cl(11)-C(31)-H(31A)	109.1
C(19)-C(24)-H(24A)	120.1(14)	Cl(12)-C(31)-H(31A)	109.1
C(26B)-C(25)-C(26A)	54.5(3)	Cl(13)-C(31)-H(31B)	97.9
C(26B)-C(25)-N(1)	120.9(3)	Cl(11)-C(31)-H(31B)	109.1
C(26A)-C(25)-N(1)	118.8(2)	Cl(12)-C(31)-H(31B)	109.1
C(26B)-C(25)-H(25A)	131.2	H(31A)-C(31)-H(31B)	107.9
C(26A)-C(25)-H(25A)	107.6	Cl(13)-C(31)-H(31C)	112.3
N(1)-C(25)-H(25A)	107.6	Cl(11)-C(31)-H(31C)	110.5
C(26B)-C(25)-H(25B)	54.6	Cl(12)-C(31)-H(31C)	121.6
C(26A)-C(25)-H(25B)	107.6	H(31A)-C(31)-H(31C)	91.8
N(1)-C(25)-H(25B)	107.6	Cl(13)-C(31)-H(31D)	105.6
H(25A)-C(25)-H(25B)	107.1	Cl(11)-C(31)-H(31D)	110.4
C(26B)-C(25)-H(25C)	107.1	Cl(12)-C(31)-H(31D)	91.4
C(26A)-C(25)-H(25C)	55.2	H(31B)-C(31)-H(31D)	123.2
N(1)-C(25)-H(25C)	107.1	H(31C)-C(31)-H(31D)	108.7
H(25A)-C(25)-H(25C)	60.1	Cl(22)-C(32)-Cl(21)	113.71(16)
H(25B)-C(25)-H(25C)	145.2	Cl(21)-C(32)-Cl(23)	110.42(18)
C(26B)-C(25)-H(25D)	107.1	Cl(22)-C(32)-H(32A)	108.8
C(26A)-C(25)-H(25D)	133.7	Cl(21)-C(32)-H(32A)	108.8
N(1)-C(25)-H(25D)	107.1	Cl(23)-C(32)-H(32A)	90.6
H(25A)-C(25)-H(25D)	48.5	Cl(22)-C(32)-H(32B)	108.8
H(25B)-C(25)-H(25D)	60.9	Cl(21)-C(32)-H(32B)	108.8
H(25C)-C(25)-H(25D)	106.8	Cl(23)-C(32)-H(32B)	127.8
O(1)-C(26A)-C(25)	110.3(2)	H(32A)-C(32)-H(32B)	107.7
O(1)-C(26A)-H(25C)	146.8	Cl(22)-C(32)-H(32C)	88.9
O(1)-C(26A)-H(26A)	109.6	Cl(21)-C(32)-H(32C)	109.6
C(25)-C(26A)-H(26A)	109.6	Cl(23)-C(32)-H(32C)	109.9
H(25C)-C(26A)-H(26A)	75.1	H(32A)-C(32)-H(32C)	125.7
O(1)-C(26A)-H(26B)	109.6	Cl(22)-C(32)-H(32D)	124.3
C(25)-C(26A)-H(26B)	109.6	Cl(21)-C(32)-H(32D)	109.5
H(25C)-C(26A)-H(26B)	99.3	Cl(23)-C(32)-H(32D)	109.4
H(26A)-C(26A)-H(26B)	108.1	H(32B)-C(32)-H(32D)	87.9
O(1)-C(27A)-H(27A)	109.5	H(32C)-C(32)-H(32D)	108.1

Symmetry transformations used to generate equivalent atoms: #1 -x+2,-y+1,-z+2

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Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for 5 (CCDC 258068). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cr(1)	146(1)	168(1)	161(2)	-8(1)	54(1)	10(1)
Cl(1)	200(2)	197(2)	221(2)	23(2)	67(2)	44(2)
Cl(2)	179(2)	222(2)	269(3)	-15(2)	35(2)	-19(2)
Cl(3)	179(2)	194(2)	176(2)	5(2)	73(2)	32(2)
P(1)	183(2)	193(2)	201(3)	20(2)	91(2)	34(2)
P(2)	171(2)	201(2)	177(3)	-24(2)	55(2)	4(2)
O(1)	413(9)	553(10)	206(9)	-80(7)	-12(7)	202(8)
N(1)	196(8)	237(8)	180(8)	-47(7)	69(6)	7(6)
C(1)	186(9)	169(9)	288(11)	59(8)	131(8)	31(7)
C(2)	300(12)	319(12)	324(14)	21(10)	163(10)	62(9)
C(3)	315(12)	296(12)	492(16)	-33(11)	241(12)	66(9)
C(4)	197(11)	229(11)	556(16)	75(10)	170(11)	48(9)
C(5)	192(10)	311(11)	347(14)	91(10)	84(10)	0(9)
C(6)	225(10)	266(10)	328(13)	25(9)	141(9)	8(8)
C(7)	250(10)	219(9)	233(11)	13(8)	147(8)	64(8)
C(8)	358(13)	282(11)	235(12)	19(9)	97(10)	45(10)
C(9)	537(16)	308(12)	251(13)	74(10)	126(12)	139(11)
C(10)	590(16)	247(11)	409(15)	115(10)	336(13)	109(11)
C(11)	364(13)	264(11)	495(16)	81(10)	263(12)	29(10)
C(12)	252(11)	279(11)	370(13)	86(10)	159(10)	67(9)
C(13)	250(10)	200(9)	173(10)	-59(8)	54(8)	-25(8)
C(14)	247(11)	278(11)	270(12)	-48(9)	73(9)	-7(9)
C(15)	317(12)	299(12)	387(14)	-113(10)	112(10)	-124(10)
C(16)	480(15)	240(11)	329(13)	-57(10)	93(11)	-88(10)
C(17)	323(12)	238(11)	294(13)	-31(9)	36(10)	21(9)
C(18)	241(11)	235(10)	212(11)	-38(8)	33(8)	-21(8)
C(19)	159(9)	181(9)	272(11)	-40(8)	51(8)	4(7)
C(20)	268(12)	442(13)	304(13)	27(10)	112(10)	113(10)
C(21)	327(13)	473(14)	342(15)	113(12)	54(11)	105(11)
C(22)	178(11)	277(11)	544(16)	-10(10)	107(10)	36(9)
C(23)	216(11)	377(12)	433(15)	-89(11)	149(10)	-7(9)
C(24)	215(10)	363(12)	280(13)	-68(10)	90(9)	-26(9)
C(25)	435(13)	322(11)	240(12)	-49(9)	145(10)	91(10)
C(26A)	330(20)	340(20)	185(18)	-30(14)	65(15)	131(16)
C(27A)	420(20)	670(30)	280(20)	-130(20)	117(19)	-120(20)
C(26B)	300(30)	270(30)	280(30)	-70(20)	100(20)	-30(20)
C(27B)	400(40)	480(40)	280(30)	60(30)	120(30)	90(30)
C(31)	435(14)	302(12)	447(15)	-52(11)	94(12)	53(10)
Cl(11)	696(4)	395(3)	501(4)	-26(3)	207(3)	-103(3)
Cl(12)	305(12)	390(15)	557(17)	-125(9)	86(10)	-39(10)
Cl(13)	435(14)	990(30)	1050(60)	-380(30)	-90(20)	275(17)
C(32)	420(15)	601(17)	495(17)	-85(14)	90(12)	141(13)
Cl(21)	384(3)	423(3)	689(5)	85(3)	228(3)	46(3)
Cl(22)	310(8)	610(20)	690(20)	-305(15)	121(9)	2(9)
Cl(23)	412(10)	666(19)	692(14)	210(17)	-12(9)	66(11)